ENHANCEMENT TO HITRAN TO SUPPORT

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Abstract— The HITRAN molecular database has been enhanced with the object of providing improved capabilities for the **EOS** program scientists. HITRAN itself is the database of high-resolution line parameters of gaseous species expected to be observed by the **EOS** program in its remote sensing activities. The database is part of a larger compilation that includes IR cross-sections, aerosol indices of refraction, and software for filtering and plotting portions of the database. These properties have also been improved. The software has been advanced in order to work on multiple platforms. Besides the delivery of the compilation on CD-ROM, the effort has been directed toward making timely access of data and software on the world wide web.

keywords: Absorption, Atmosphere, Emission, HITRAN, IR Cross-sections, Radiance, Remote Sensing, Spectroscopy

1. Introduction

The purpose of this project is to develop and enhance the HITRAN molecular spectroscopic database and associated software to support the observational programs of the Earth Observing System (**EOS**). In particular, the focus is on the EOS projects: the Atmospheric Infrared Sounder (**AIRS**), the High-Resolution Dynamics Limb Sounder (**HIRDLS**), Measurements of Pollution in the Troposphere (**MOPITT**), the Tropospheric Emission Spectrometer (**TES**), and the Stratospheric Aerosol and Gas Experiment (**SAGE** III). The data requirements of these programs in terms of spectroscopy are varied, but usually call for additional spectral parameters or improvements to existing molecular bands. In addition, cross-section data for heavier molecular species must be expanded and made amenable to modeling in remote sensing. The effort in the current project also includes developing software and distribution to make access, manipulation, and use of HITRAN functional to the EOS program.

2. HITRAN Data Improvement

The effort to improve, enhance, and extend the HITRAN database continued at several levels. For the line-by-line portion of the compilation, the EOS observational requirements may be for completely updated spectroscopic parameters, including line positions, intensities, halfwidths, and temperature dependence coefficients. Often improving a subset of the parameters that are deficient may be sufficient at this time, such as the air-broadened halfwidth if that is causing a problem for adequate modeling. From discussions with the teams of the EOS experiments, one also wants to anticipate future requirements so that a heads-up approach is taken. This often takes the form of adding new bands for existing molecules (overtones and combination bands), adding new molecular absorbers that are trace constituents of the atmosphere, and completing spectroscopic parameters for the transitions (such as pressure-shift,

etc.). Another major thrust of the data improvement of the compilation is the incorporation of absorption cross-sections. Unlike the line-by-line traditional HITRAN parameters, these data are used primarily for molecules with extremely dense spectra, such as the chlorofluorocarbons and "heavy" oxides of nitrogen. With recent advances in atmospheric modeling using the HITRAN format of cross-sections, the EOS community has benefitted from this approach.

Discussions and recommendations were made with Curtis Rinsland of NASA Langley Research Center with regard to IR updates to make for ozone on the next edition, HITRAN 2000. A summary of the changes recommended for changing the air-broadened widths, the air-broadened shifts, and the temperature-dependence (η) of the air-broadened halfwidth are given here:

1. ν_2 band — Adopt the mean value of η(air) = 0.53 ± 0.08. Adopt the mean air shift (δ) of -0.0008 cm^{-1}/atm at 296 K. These values are from the Malathy Devi et al, *J.Mol.Spectrosc.* **182**, 221-238 (1997).

2. ν_1 band — Adopt the mean value of η(air) = 0.67 ± 0.07. Adopt the mean air shift of -0.0007 cm^{-1}/atm at 296 K. These values are from M.A.H.Smith et al, *J.Mol.Spectrosc.* **182**, 239-259 (1997).

3. $\nu_1+\nu_2+\nu_3$ band — Adopt a mean air shift of -0.004 ± 0.004 cm^{-1}/atm at 296 K. This value comes from Table IV of M.A.H. Smith et al, *J.Mol.Spectrosc.* **164**, 239-259 (1994).

4. $3\nu_3$ band — Adopt a mean air shift of -0.008 ± 0.003 cm^{-1}/atm at 296 K. This value also comes from Table 4 of M.A.H. Smith et al, *J.Mol.Spectrosc.* **164**, 239-259 (1994).

These are modest changes. Of course, we could introduce the individual measurement values, but mean values should be reasonable for this round. Rinsland had recommended that the other parameters remain at the HITRAN defaults. He is also planning to proceed with the O_3 lab run at Denver this summer, and is hoping to get someone from the laboratory of Jean-Marie Flaud

and Agnès Perrin in Orsay, France to visit NASA and work on the data. The plan is to cover the IR at 0.001 cm^{-1} resolution, a major improvement over their earlier lab data.

Rinsland is working with Rothman on including UV parameters for ozone. We are also evaluating other updates based on GEISA97 ("The 1997 spectroscopic GEISA databank," N. Husson et al, *J. Quant. Spectrosc. and Rad. Transfer* **62**, 205-254 (1999)) and other studies that have taken place in various international laboratories involved in ozone lab measurements and consistent fitting of parameters (establishments like the University of Reims, France; JPL; and the DLR - German Aerospace Research - near Munich).

Many sets of data, constants, and fitting programs were received from Prof. William Blass of the University of Tennessee concerning his effort to determine the spectra of ethane (C_2H_6). We have examined these files and find that they will require a great deal of work to cast into a form acceptable to the HITRAN database.

Discussions with Ed Pearson (TASC, Reading MA) have indicated that there are inversion lines of ammonia missing from HIRAN, especially around 24 GHz extending to 40 GHz. Lines currently end at about .5cm-1. We will examine the JPL catalog, and consult with Petr Pracna (Czech Academy of Sciences) and Linda Brown of JPL concerning this issue.

2.1 Teleconference: Our first telecon for the UV cross-sections for the next edition of the HITRAN compilation (HITRAN2000) was focused only on discussing the ozone molecule. Participating in the discussion were Rothman, Kelly Chance, Bill Parkinson, Kouichi Yoshino (SAO), Eric Shettle (NRL), Curt Rinsland (NASA Langley), and Aaron Goldman (University of Denver). The scope of our discussions are to: 1) decide what data is available, 2) how to proceed to assemble them, 3) decide what data sets to incorporate into HITRAN, and less urgently 4) consider more long-range plans to improve on these data. The series of teleconferences have

been organized through the auspices of NASA Langley and have been an extremely cost-effective means of making progress for the HITRAN program.

We first agreed that the format for the datasets would follow the standard already established in HITRAN (see Table 9 of the current article). We will, however, try to standardize slightly more the last part of the header in terms of the reference pointer *and* putting the experimental resolution there. The formatting for the UV entails converting the measurements into wavenumber, as has been done already for the two molecules in the UV in HITRAN96.

I. Hartley-Huggins bands

At the moment we propose to take the GOME (Global Ozone Monitoring Experiment) FM measurements at 5 temperatures (203 to 293K), the portion that is the Hartley-Huggins bands (237 to 407nm), convert them to a wavenumber scale and see if we can improve them with the Bremen FTS measurements. We will await the visit of Johannes Orphal here and we expect that the process will take about a day. If it is not an improvement, we will use the FM data in HITRAN, and if it is an improvement we will use the amalgam of the two. We will also provide the URL for obtaining the quadratic parametrization of the temperature-dependence of the cross-sections.

II. Chappuis and Wulf bands

The default for HITRAN2000 will be the subroutine by Eric Shettle (NRL) and Stu Anderson. Eric may improve on it in the coming months, but we will assume that what we have is what you get in HITRAN2000. The data referenced in the subroutine should be crossed checked against the results for traceability.

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Eric Shettle had some additional comments on the telecon related to the Hartley-Huggins bands:

1) Given the Bass & Paur cross sections are the defacto standard used by the ozone community making UV measurements, [TOMS, SBUV, ground-based Dobson, Umkehr, & Brewer measurements, and the UV lidars], if we put forward any other data set over the 230 to 330 nm range, we need to show it is clearly better than Bass & Paur.

2) In addition to the Bremen GOME & FTS data, we should look at the University of Reims data, which covers from 195 to 345 nm, with T = 218 to 295 K, a resolution of 0.02 nm. [Daumont et al., *J Atmos. Chem* **15**, 145-155 (1992); Brion et al, *Chem. Phys. Lettr* **213**, 610-612 (1993); and Malicet et al, *J. Atmos. Chem.* **21**, 263-273 (1995)]. The room temperature data has been extended from 345 to 830 nm, with data at 218 K from 515 to 650 nm, by Brion et al, *J. Atmos. Chem.* **30**, 291-299 (1998).

3) Properly, the dividing point between the Huggins & Chappuis bands should be around the minimum between them. Burrows et al puts the dividing point at 370 nm and Brion et al at 375 nm. Until the Chappuis band data is extended from 407 nm to shorter wavelengths, there is a practical issue of filling the gap. Whatever is used from 370 nm to 407 nm needs to merge smoothly into the Chappuis band data at longer wavelengths, as well as merge smoothly into the UV data at shorter wavelengths. Hopefully we will be able to use the same data set continuously from the UV through the visible, but right now that is not necessarily the case.

2.2 Meetings: There were two major meetings that were attended during the month of June, the *54th Ohio State University International Symposium on Molecular Spectroscopy*, 14-18 June in Columbus, Ohio and the combined Optical Society of America topical meetings, *Fourier Transform Spectroscopy: New Methods and Applications* and *Optical Remote Sensing of the Atmosphere*, 22-24 June in Santa Barbara, California. The period between these two meetings allowed a convenient visit with collaborators at JPL. We also attended the session on *Atomic*

and Molecular Processes in the Atmospheres of the Earth, Planets, and Comets II, presided by Alex Dalgarno of the Harvard-Smithsonian center for Astrophysics, at the Spring Meeting of the American Geophysical Union held in Boston 1-4 June.

The Ohio State Symposium is the pre-eminent conference on molecular spectroscopy in the world. It provides a very fertile ground for assimilating new and improved data for the HITRAN program. It also affords the chance to have discussions with many of the US and international contributors to HITRAN in one setting.

The presentations at the Ohio State meeting are all oral. Among the most relevant presentations and information gleaned relevant to the HITRAN program were the following:

-- Paper WH01, "The Intensities of Methane in the 3μm Region Revisited," by Linda Brown. A good history of the CH_4 parameter history was given, and the theory (also shown in Rao and Weber's book) was reviewed. Besides the update, corrections for strengths and positions of this pentad system were given. Linda also discussed new ammonia replacements as well as replacements for the three isotopomers of methane in HITRAN.

-- Paper WH03, "Measurements of Air-broadening and Pressure-shift Coefficients and Line-mixing in the v_6 Fundamental Band of $^{12}CH_3D$," presented by V.Malathy Devi (College of William and Mary) with C.P. Rinsland, M.A.H. Smith (NASA Langley) and Linda Brown. The results of this investigation must be put into the next HITRAN.

-- Paper WH04, "Air-broadening and Shift Coefficients and Line-mixing in the v_3 Band of $^{12}CH_3D$," presented by M.A.H. Smith with V.Malathy Devi, C.P. Rinsland, and Linda Brown. Similar to the previous paper, the results of this investigation must be put into the next HITRAN. They have an empirical fit of coefficients resulting in a convenient algorithm for the air-broadened halfwidths,

$$\gamma_{air} = \gamma_0 + \gamma_1 J(J+1) + \gamma_2 f(K).$$

Two invited papers were given in a session on Spectroscopy and Environmental Monitoring:

– Paper RB01, "Optical Spectroscopic Techniques for Army Applications," presented by Kevin McNesby, US Army Research Laboratory. Especially relevant to HITRAN is the need for more current data on CF_3Br.

– Paper RB02, "Observation and Analysis of the Water Absorption Spectrum from Near IR to Near UV Region," by Peter Bernath (University of Waterloo) and co-workers. The effort here is of great interest to the HITRAN program, not only for standard atmospheric remote sensing programs, but for higher temperature applications, such as applied to some TES observations. The group involved with this research includes a group at University College London under the supervision of Jonathan Tennyson (who was a visiting scientist at the SAO for one year), and experimental teams in Brussels and in Reims, France. We will be forging an alliance with this team for updating, identifying, and developing new water-vapor parameters. Incidental to this talk, Bob Sams (Battelle Pacific Northwest laboratories) commented that he has measured new water-vapor parameters in the 7000 cm^{-1} region and possibly has information on the continuum there.

– Paper RI01, "High Vibrational Levels and Potential Energy Curves for the O_2 b$^1\Sigma$, a$^1\Delta_g$, and X$^3\Sigma$ States Derived from Atmospheric Nightglow Emissions," presented by D.L. Huestis, SRI International. This paper (which was also heard given by co-author T.G. Slanger at the Spring Meeting of the American Geophysical Union held in Boston) is a major improvement resulting from observations and analyses of emissions taken with the 10-m Keck telescope and HIRES spectrograph. Knowledge of higher-level vibrational states is now available, many of which have been only available from low-resolution, old spectra heretofore in HITRAN.

– Paper FB01, "High Resolution Analysis of H2CO in the 3.6 and 4.3μm Region by Fourier Transform Spectroscopy," presented by Agnès Perrin and co-workers (University of Paris). We are about to obtain these data from the French. At the meeting, Bob Sams warned about the problem of determining strengths for these data using ratios, and also of the many blended lines. There are A-, B-, and C-type interactions that all have to be considered.

I assembled several colleagues present at the Ohio State conference for an ad hoc meeting on the future of HITRAN. Attending were Linda Brown, Mary Ann Smith, V. Malathy Devi, D. Chris Benner (College of William and Mary), Robert Gamache (Univ. of Mass at Lowell), and Agnès Perrin. We started by discussing the proposed new format for the next edition of HITRAN. There was mostly agreement with my proposal, although some sentiment for adding more parameters for self-interactions (temperature dependence of the broadening, shift, and references). There was also some discussion of adding parameters for planetary studies, such as hydrogen and helium broadening. We then went down the list of HITRAN molecules in their chronological order.

– Much time was allotted to the first, water vapor. We need to press for incorporation of the work of Laurent Coudert (University of Paris) in the v_2 region. This is being done with Ken Jucks at SAO. In the 600-2000 cm^{-1} and 6000-9000 cm^{-1} regions, the measurements of Bob Toth (JPL), who has also observed the isotopes, must be taken into account. There has been problems in getting the data, and we have asked Linda Brown and Curtis Rinsland to pursue avenues.

– For carbon dioxide, Chris Benner will send his data in the 3300 to 4000 cm^{-1} region. These data represent a big improvement over the older grating spectrometer data that are still being used here by HITRAN. We are also obtaining new results for band intensities for some bands in

the shorter wavelength region taken in the laboratory by Larry Giver at NASA Ames Research Center.

– For ozone, we can at least use mean shift data for the high-vibrational bands, and it was emphasized that the UV cross-sections should be made available.

– For N_2O, we again need to obtain the improved data from Bob Toth in the 4000 - 5000 cm^{-1} region.

– For carbon monoxide, we will update parameters based on the work of Chuck Chackerian (NASA Ames)

– Methane will be updated by Linda Brown.

– For oxygen, we will update the strength of the $a^1\Delta_g$ band (1.27 µm) and Linda will supply new data for the A-band.

– For NO, the halfwidths will be updated and made self-consistent.

– For OH, Aaron Goldman (University of Denver) is supplying new parameters

– For SO_2, we will follow newer work at the University of Paris by Perrin.

– For NO_2, the hot band will be re-visited, and we will apply the halfwidth algorithm provided by Victor Dana (University of Paris).

– For ammonia, Linda Brown will provide a replacement for the 3- and 6-µm regions and has suggested that we use the halfwidths determined by Vasily Nemtchinov (JPL, measurements made while a graduate student at SUNY Stony Brook).

– For HNO_3, we need some re-scaling of intensities.

– For HCl, Rinsland will provide updated positions.

– For HBr, we will use the newer data as published by Mike Coffey (NCAR) et al.

– A ClO update can be provided by Rinsland.

– H_2CO has been discussed by Perrin in her presentation at the meeting.

– For HOCl, we need to consult with Jean-Marin Flaud (University of Paris) regarding the status of parameters for both pure rotation and the ν_2 band.

– For CH$_3$Cl, Linda may have improved widths and has looked at the band around 730 cm^{-1}. E. Pearson has already brought up the need for pure rotation lines in a communication to me in May.

We also have the need for bands at 1000 cm^{-1} and 13-1500 cm^{-1} (a communication from Jim Wray, Optical Physics Company, California).

– For H$_2$O$_2$, Kelly Chance (SAO) has provided far infrared parameters, but we need broadening.

– For ethane, C$_2$H$_6$, Goldman can scale Steve Daunt's data for improvement. Alan Pine's data taken when he was at NIST may also be incorporated according to Rinsland.

– For H$_2$S, Linda now has new 2.7- and 4-μm data.

– For HCOOH, Goldman has improvements.

– It was agreed that at this time, chlorine nitrate (ClONO$_2$) parameters should be moved out of the main portion of HITRAN and users should be encouraged to use the cross-sections instead.

– Conversely, HOBr parameters should be moved from the current supplemental directory to the main part of HITRAN.

– We also discussed adding new species such as acetone (CH$_3$COCH$_3$), propane (C$_3$H$_8$), methanol (from measurements made at the University of New Brunswick by Li-Hong Xu and also presented at the last HITRAN meeting), and methyl bromide (CH$_3$Br).

At the joint Optical Society of America meeting in late June, I again found that although I registered for the Remote Sensing of the Atmosphere meeting, the Fourier Transform Spectroscopy meeting had many more papers of interest, and in fact was much better organized. Of particular interest was the paper "Laboratory Spectroscopy of Molecular Oxygen in the

Visible and Near-infrared," presented by Roland Schermaul of the Imperial College of science, Technology and Medicine, London UK. He has developed a far more rigorous development of the Honl-London factors for the oxygen $a^1\Delta_g$ band. He anticipates having data soon on the pressure-induced band as well.

3. PUBLICATIONS

During this period we published the HITRAN Newsletter. The Newsletter was placed in the HITRAN web-site in pdf format. This was the first time we distributed it electronically, rather than by hard copy. A broad announcement was made via e-mail to the HITRAN user-list. The feedback that we had was encouraging.

The cover pages of three publications since the last annual report are given below. The GEISA database is essentially a copy of the HITRAN database, but includes some species of planetary interest since that was the database's original goal (created for the NASA Voyager missions). However, due to the timing of publication of database archives, there are some more updated data on this database, and as we have mentioned, ozone in particular needs examining for HITRAN. The paper by Gamache et al was submitted to the *Journal of Molecular Structure* for a special issue commemorating the 65th birthday of Prof. Georges Graner. As we await the publication, one wonders if it will commemorate his 100th. There has also been a long delay for the publication of the article by Goldman et al. These latter two articles highlight the methodology and calculations that must go into a thorough treatment of partition sums for the HITRAN molecules. The next edition of HITRAN will introduce the Einstein-A coefficient and the upper and lower statistical weights of the levels. The partition sums, especially for the

diverse types of symmetries in HITRAN and the fact that some lines possess hyperfine splitting, takes on an important role in atmospheric simulations and modeling.

The 1997 spectroscopic GEISA databank

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ELSEVIER

Total internal partition sums for molecules in the terrestrial atmosphere

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Abstract

Total internal partition sums (TIPS) are calculated for most of the infrared-absorbing molecules in the terrestrial atmosphere. The list includes the principal isotopic species and many of the lesser abundant isotopomers. The calculations are made for temperatures from 70 to 3005 K. The temperature range is divided into three regions and the resulting TIPS are fit to a third-order polynomial expression for later rapid recall of the total partition sum, $Q(T)$. The method of calculation of $Q(T)$ for each isotopomer, convergence of the partition sum in each temperature range, the quality of the fit of the data, and comparisons with other work are discussed. © 1999 Elsevier Science B.V. All rights reserved.

Keywords: Total internal partition sums; Partition functions; Atmospheric molecular species; HITRAN; Temperature dependence of partition function

1. Introduction

The knowledge of the total internal partition sum (TIPS) is useful for a number of reasons. For a system in thermodynamic equilibrium, the states obey a Boltzmann distribution. Hence the number density of molecules each in a particular state at a given temperature and pressure can be obtained from the total internal partition function at that temperature. Relationships between the intensity of a spectral line and the transition-moment squared, or the Einstein A coefficient, or the oscillator strength require that the partition sum be known [1,2]. If the intensity of a

spectral line is known, the intensity at other temperatures can be obtained knowing the partition sum at both temperatures. This has important consequences when studying systems that are not isothermal, e.g. the terrestrial atmosphere. Having a database of spectral lines of all the important atmospheric species [3,4] and knowing the partition sum at atmospheric temperatures, atmospheric spectra can be inverted to obtain concentration profiles. Note, in the literature, the term partition function is synonymous with the term partition sum.

In this paper, we present the calculations of the total internal partition sums for many of the molecular isotopomers that absorb infrared radiation in the terrestrial atmosphere. The list of species is taken from the 1992 HITRAN database [5] with three additional species from the 1996 HITRAN database [3]. These are shown in column one of Table 1. However,

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HITRAN Partition Functions and Weighted Transition-Moments Squared

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Abstract

The calculations of the partition functions and weighted transition-moments squared in the HITRAN database are reviewed. It was found that for several of the HITRAN molecules corrections are needed to the partition functions. Corrections to the weighted transition-moments squared are needed for most of the HITRAN molecules. Replacement of the weighted transition-moments squared by other quantities is proposed.

1 Introduction

The 1996 HITRAN database[1] provides improved polynomial representation for the partition functions of the isotopomers represented in the database.[2–4] These include results from the recent work of Gamache et al[4] where the initial work for linear molecules (Gamache et al[2]) was extended to the complete set of the HITRAN 1996 molecules. The database also includes weighted transition-moments squared (proportional to the weighted transition probabilities) for most of the listed transitions.[5] However, on close inspection, the need for several types of corrections has been observed in both quantities.

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HITRAN NEWSLETTER, July 1999

1. HITRAN/HITEMP has moved to the Harvard-Smithsonian Center for Astrophysics

This HITRAN newsletter marks the first one in the Adobe® PDF (Portable Document File) electronic format distributed via the HITRAN web-site (www.HITRAN.com). We are also making the text portions available as a PDB file for users who have a 3Com Palm® Pilot.

The past year, 1998, has witnessed several significant milestones and changes for the HITRAN database. It was the 25th anniversary of the first public release of the molecular database. This event was celebrated at the conference held in September at Hanscom AFB which is described elsewhere in this newsletter.

February 1999 marked a change of address for HITRAN with the move of Larry Rothman to the Smithsonian Astrophysical Observatory at Harvard University. This move will make available new and important data to support the increasing needs of the user community. HITRAN will continue to support the requirements of the atmospheric remote sensing and radiative transfer modeling communities as well as address the needs of anticipated new users. Toward this objective, a major effort is underway for a new database edition, HITRAN2000.

Dr. Rothman will maintain his relationship with the Air Force Research Laboratory through an emeritus position and will continue to provide the molecular, aerosol, and cross-section data used by atmospheric modeling codes, such as MODTRAN and FASCODE.

New information you should add to your mailing list:

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2. HITRAN Documentation on the HITRAN Web-site

The HITRAN web-site (www.HITRAN.com) continues to be an important method to distribute information related to the database. This newsletter is now being distributed via the web in the Adobe® Portable Document File format. PDF files can be viewed on most computer platforms (e.g., MAC, UNIX, MS Windows) using the appropriate reader. These readers are provided by Adobe at no charge and can be downloaded from their web-site. A link to this site is provided in the HITRAN web-site.

In addition to the newsletter, two other documents, in PDF format, are available via the web-site. The first is the user manual for the HAWKS (HITRAN Atmospheric Workstation) software. The second is a preprint of the article on the HITRAN compilation *(Journal of Quantitative Spectroscopy and Radiative Transfer*, volume **60**, pp.665-710 (1998)). The latter is the definitive description of the data contained in the CD-ROM.

The 1996 HITRAN CD-ROM contained software, called HAWKS, provided to enable users to extract data from the database; sort and merge data in the HITRAN format; plot the data; and perform statistical calculations on the vibrational/rotational bands. In addition, the software allowed the user to read abstracts of technical papers relevant to the line positions, half-widths, and intensities of the molecular data.

A comprehensive user manual is provided with the HAWKS software. It is designed to assist the user in easily adapting to the manipulation of the HITRAN96 molecular spectroscopic database

and associated molecular databases by proper utilization of the HAWKS software package. It includes installation instructions for the Windows and UNIX software, and a detailed description of the capabilities of the HAWKS software.

Two versions of the manual are provided on the CD-ROM in the DOCUMENT directory in a PKZIP executable file format. The first, called HAWKS_WP.EXE, contains the manual in the Corel WordPerfect® format. The second, called HAWKS_PS.EXE, contains the manual in an Adobe Postscript® format. A user can expand these files by copying them into the desired directory on his hard disk and typing the file name. A document file and several linked image files will be generated for the former, while a large Postscript file will be produced for the latter. Unfortunately neither of these is particularly easy to read and print. Consequently, a third version is available on the HITRAN web page in the Adobe Acrobat® (PDF) format. The document, along with a reader, can be easily downloaded. Those users who wish to make a printed copy of the manual are encouraged to use this version.

3. New HAWKS Software

A major upgrade of the HAWKS software is nearing completion. The 1996 HITRAN CD-ROM included two versions of the HAWKS software, one for systems using MS Windows (3.1, 95, 98, and NT), and a second version for SUN Solaris 2®, and SUN OS 4®. (There is a slightly updated version of HAWKS.EXE located in the web-site.) On the 1996 CD-ROM, there is no version for other operating systems such as MACs, VAX, or other UNIX computers, although generic software is provided that can be compiled and run. The generic software lacks some of the more user-friendly features of the Windows versions.

The new software is being written in the JAVA programming language and will be a complete cross-platform application. That is, the same executable code will run on a PC, UNIX workstation, and Macintosh computers. This is a significant improvement because we will only need to maintain a single source and executable code compared to the several versions we currently maintain. We will have thus greatly reduced difficulties with version control.

In addition to the capabilities of the current HAWKS, the new software will have new options for writing files, and will let the user select and plot cross-section data.

We have tested the software on PC, UNIX, and MAC platforms and are encouraged by the results. The Java version is slower than the older C software, because of the nature of Java. The speed difference as of March 1999 is about a factor of five. However, over the past year, the speed of Java has increased by approximately a factor of three, and the speed is just at the limit of acceptability. We anticipate that a combination of increased processor speeds, and improvements to Java will shortly make the speed more than adequate for most users.

The new software is also designed to run over the web. Toward the end of 1999 users will be able to select and download HITRAN data via the web using the new software. The software will be distributed via the HITRAN web-site so users are encouraged to check the web-site from time to time for its availability.

4. Twenty-fifth Anniversary HITRAN Database Conference

On 23-25 September 1998, the fifth in a series of conferences on the HITRAN molecular database and related issues was held at the Air Force Research Laboratory at Hanscom AFB, Massachusetts. This meeting celebrated the 25th anniversary of the first public release of HITRAN (on magnetic tape) in 1973. The keynote speaker was Prof. Richard Goody, former director of the Planetary and Applied Physics Department at Harvard University, and now Professor Emeritus at Harvard. His book, "Atmospheric Radiation, Vol. I Theoretical Basis," published in 1964, had a seminal impact on the creation of the HITRAN database.

There were five sessions: 1) Molecules and Cross-sections; 2) Line-mixing; 3) Databases; 4) Aerosols; and 5) Applications. In addition to invited papers on these subjects, there was also a poster session. The abstracts of the oral and poster presentations can be viewed in the HITRAN web-site using a link in the page "Latest News." At the conclusion of the meeting, an open panel session was held to summarize the findings of the conference and to formulate the priorities and future direction of the next HITRAN edition. Some of the more significant decisions were: the methodology to parametrize line-mixing (line-coupling), the substitution of the Einstein-A coefficient for the current transition-moment squared, and an increase in the number of parameters describing an individual transition.

Line-coupling produces an apparent distortion in the half-widths of some densely packed lines. This effect can cause a pronounced effect on atmospheric remote sensing. Attempts had been made on a past HITRAN database (the edition of 1986) to parametrize line-coupling for key carbon dioxide Q-branches that were being used for retrievals. However, the simple first-order theory employed at the time gave rise to great errors in some simulations. Jean-Michel Hartmann (University of Paris) and co-workers have now come up with a scheme that satisfies many previous problems: it can be adapted to many absorbing species, minimizes the amount of data that has to be stored, is quite maintainable when changes are made to other related parameters on the database, minimizes changes to subsequent modeling codes, and minimizes risks of misuse.

The current edition of HITRAN uses a parameter, the weighted transition-moment squared. This parameter is similar to the line intensity on the database, but is independent of temperature and isotopic ratio, and was added to the database initially for the purpose of aiding codes concerned with non-local thermodynamic equilibrium conditions. From the discussion at the meeting, as well as recent user feedback, we have decided that it would serve the community better to replace this parameter with the Einstein-A coefficient. This will also require the addition of the statistical weights for the upper and lower states of each transition.

Regrettably, the time has come again to alter the HITRAN transition format. Part of this change has been necessitated by the need for larger fields for some of the current parameters, such as the descriptors for the quantum identifications. We have more energy levels (such as in the case of CO_2 in the High Temperature database, HITEMP) or the need for greater values of rotational quanta for heavy molecules. Another issue is the request of several users to add new parameters, such as broadening by other foreign gases with the corresponding dependence on temperature.

5. Intermediate HAWKS Updates

The HITRAN web-site is being utilized for placing corrections, updates, and occasionally new data. Users should go to the sub-page called **Database Updates**. There is a slightly newer version of the MS-WINDOWS HAWKS software located there (HAWKS.EXE version number 1.1). If you use this software frequently, we recommend that you use the updated version.

We have also placed some files that were inadvertently omitted from the 1996 CD-ROM. One of these files is called MOLPARAM.TST. This file contains general information specific to all the isotopomers in HITRAN, such as statistical weights, the partition sum at 296K, isotopic abundance as used by HITRAN, and molar mass. MOL.DAT and ABUN.CMN, which are only required by some of the generic software on the CD-ROM, have also been resurrected on the web-site. Some of the other generic files have also been updated and uploaded to the web-site.

A year after the release of HITRAN96, two HITRAN-type files were deposited on the web. A file, called **38_HIT97.par**, is a compilation of parameters for ethylene (C_2H_4) in the spectral range 701 to 3242 cm^{-1}. This molecule is new to HITRAN. The second file, **19_HIT97.par**, represents a complete upgrade and replacement of carbonyl sulfide (OCS). The data are far more extensive in the IR than the older data set existing in HITRAN.

The HAWKS96 CD-ROM includes two tar (compressed) files of the HAWKS software, one for SUNOS and the other for SUN Solaris. The Solaris version will work properly up through version 2.5, but will not work for Solaris 2.6. Since we are committed to developing the cross-platform JAVA software, there are no plans to update the old software. The zApp motif windows manager file needed for the UNIX operation of HAWKS can be found in the HITRAN web-site; it was not included in the CD-ROM.

6. HITRAN Special Issue in the *JQSRT*

The 1998 November issue (volume 60, no. 5) of the *Journal of Quantitative Spectroscopy and Radiative Transfer (JQSRT)* was devoted to the HITRAN database and related issues. The lead article is the description of the current HITRAN molecular database and its associated software and data compilation (cross-sections, indices of refraction, etc). There are also articles in this Special Issue that describe the efforts behind some of the key components of the current HITRAN database. The authors report on progress, new available data, and imminent plans for the future of HITRAN. This journal is an excellent reference source for atmospheric molecular spectroscopy and associated topics. We owe our gratitude to the editor of *JQSRT*, Prof. Prasad Varanasi of the State University of New York at Stony Brook, for the encouragement he has provided in promoting focused volumes for spectroscopy and atmospheric physics in this journal.

7. Acknowledgments

8. HITRAN Advocacy

With the move of the HITRAN project from the AFRL to SAO, we are looking for new sources of support. There is a great deal of data that users would like to have added to the compilation that does not fit within the goals of the EOS and ARM programs. The program is looking for additional sponsors. Any suggestions would be appreciated.

HAWKS (HITRAN Atmospheric Workstation)

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The HAWKS (HITRAN Atmospheric Workstation) compilation includes software that allows the user to: (1) select data from a HITRAN formatted-type database; (2) display stick plots or contours of line intensities or energy levels; (3) find journal references for line positions, halfwidths, and intensities; and (4) perform other operations on HITRAN. A major upgrade of the HAWKS software is planned for release within the next year. The software is being rewritten in the JAVA programming language and will be a complete cross-platform application. That is, the same executable code will run on a PC, UNIX workstation, and Macintosh computers. This is a significant improvement because we will only need to maintain a single source and executable code compared to the four versions that are currently maintained. The software will also be distributed via the HITRAN web site.

Figure 1 illustrates the pull-down menu for the functions of manipulation of the database, namely the filtering of the line-by-line portion, HITRAN, for the required scenarios of the user. The example gives a further selection for isotopes, in this case carbon dioxide.

The plotting functionality has been substantially enhanced beyond the current edition, HITRAN96. One is now able to plot the cross-section data in addition to the line-by-line data. Figure 2a and 2b show a representative case of selecting and plotting one of the temperature-pressure sets of a chlorofluorocarbon, CFC-22 at T = 216K, P = 176 mb. Plotting can be in terms of stick plots or band contours.

There will also be capabilities for outputting the HITRAN files in a more "readable" ASCII form (a request made at the last ASA meeting).

HAWKS Select ☐		
----- Set Filenames ----		
HITRAN Filename		Output Filename
--- Selection Parameters ---		
Spectral Range		Temperature
Molecule		Band
Isotope		Cutoff
Run Select		Run Deselect
--- Batch Mode ---		
Open Batch		Save Batch
Cancel		

Figure 1. Filtering capabilities of HAWKS software. Example of isotope selection.

ction File Name D:\R_XSECT\CFC22.XSC

cted Panel CHCIF2 769.9917 Vmin 869.9950 Vmax 216.0000 K 176. mb

CHCIF2	760.0006	860.0039	9750	294.0000	760.0
CHCIF2	760.0006	860.0039	9750	273.0000	573.6
CHCIF2	760.0006	860.0039	9750	253.0000	401.1
CHCIF2	760.0006	860.0039	9750	240.0000	308.4
CHCIF2	760.0006	860.0039	9750	236.0000	270.4
CHCIF2	769.9917	869.9950	9750	216.0000	176.8
CHCIF2	760.0006	860.0039	9750	216.000x0	40.

ect File to Plot **Select Panel** **X-Axis**

Plot **Cancel** **Y-Axis**
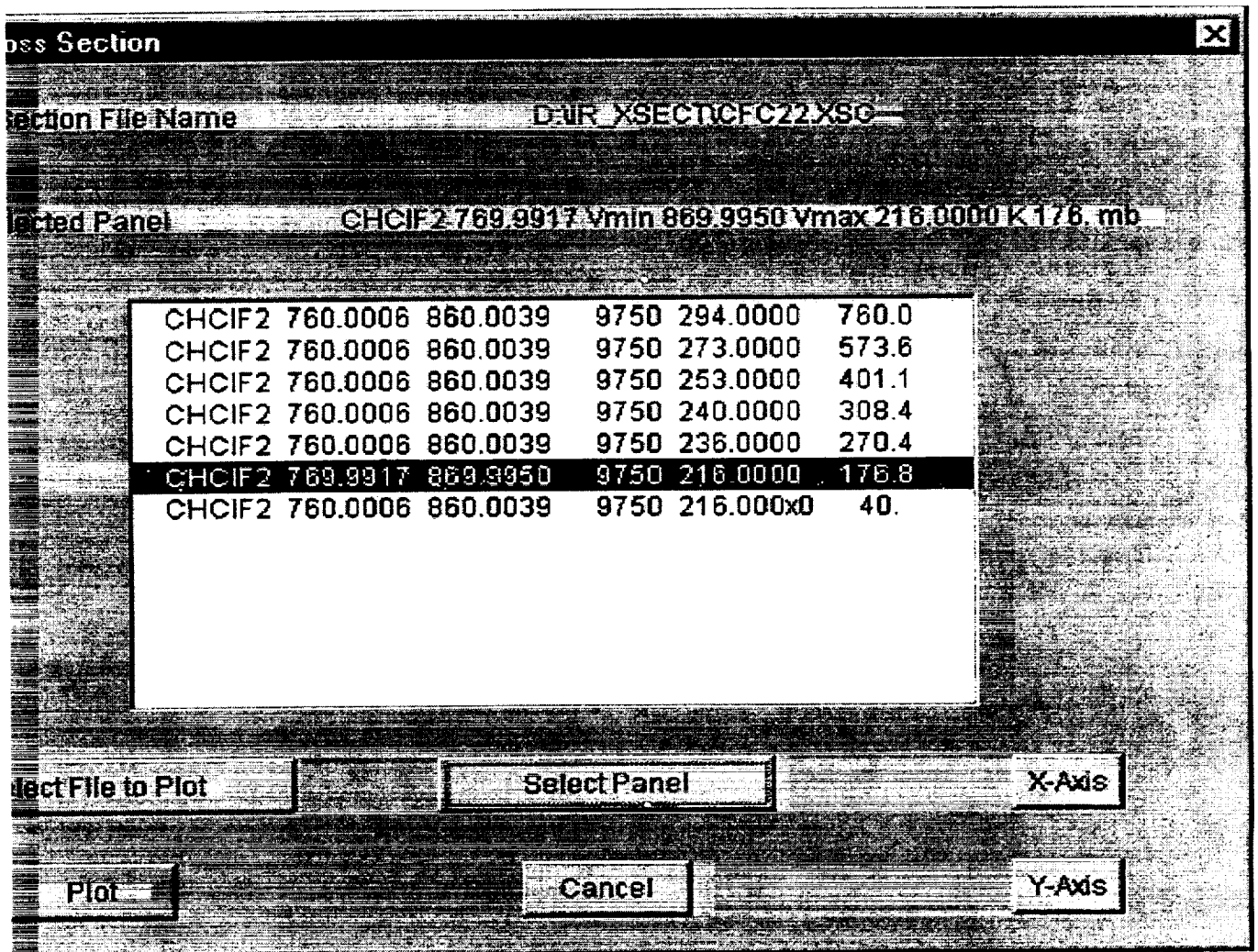
Figure 2a. Cross-section plotting selection menu.

CHCIF2 769.9917 Vmin 869.9950 Vmax 216.0000 K 176. mb
HAWKS CROSS SECTION File D:\IR_XSECT\CFC22.XSC

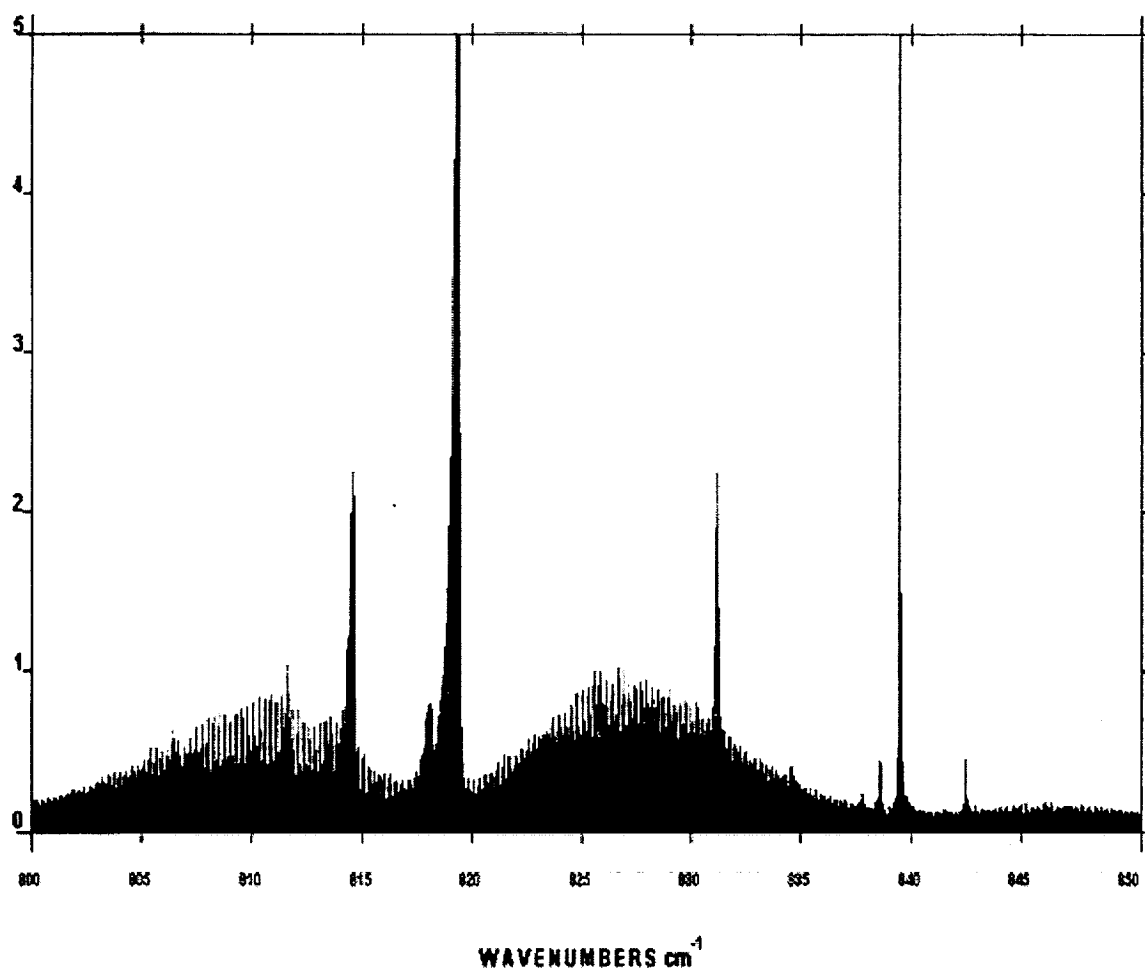**WAVENUMBERS cm^{-1}**

Figure 2b. Plot of CFC-22 at T = 216K, P = 176 mb in the spectral interval 800 to 850 cm^{-1}.

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15. Supplementary Notes

16. Abstract

The HITRAN molecular database has been enhanced with the object of providing improved capabilities for the EOS program scientists. HITRAN itself is the database of high resolution line parameters of gaseous species expected to be observed by the EOS program in its remote sensing activities. The database is part of a larger compilation which includes IR cross section, aerosol indices of refraction, and software for filtering and plotting portions of the database. These properties have also been improved. The software has been enhanced in order to work on multiple platforms. In addition to the delivery of the complilation on CD-ROM, the effort has been directed towards making timely access of data and software on the world wide web.

17. Key Words (Suggested by Author(s))	18. Distribution Statement
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